REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)

2. REPORT DATE
October 10, 1995

3. REPORT TYPE AND DATES COVERED
Technical report

4. TITLE AND SUBTITLE
Predicted Heats of Formation of DNAF in Gaseous, Liquid and Solid Phases

5. FUNDING NUMBERS
N00014-95-1-0028

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R&T Code 33e 1806

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8. PERFORMING ORGANIZATION REPORT NUMBER

85

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Office of Naval Research
Code 333
800 N. Quincy Street
Arlington, VA 22217

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release.
Unlimited distribution.

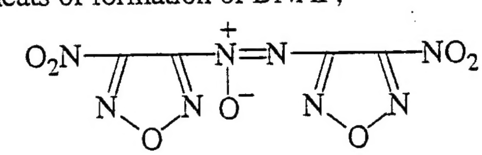
12b. DISTRIBUTION CODE

19960208 077

13. ABSTRACT (Maximum 200 words)

The predicted heats of formation of DNAF,

DNAF



based on computational analyses, are: ΔH_f(gaseous) = 169 kcal/mole = 621 cal/g; ΔH_f(liquid) = 155 kcal/mole = 570 cal/g; ΔH_f(solid) = 137 kcal/mole = 504 cal/g.

14. SUBJECT TERMS

DNAF, heats of formation

15. NUMBER OF PAGES
3

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	Unlimited

OFFICE OF NAVAL RESEARCH

CONTRACT N00014-95-1-0028

R&T Code 33e 1806

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Technical Report No. 85

PREDICTED HEATS OF FORMATION OF DNAF IN GASEOUS, LIQUID AND SOLID PHASES

by

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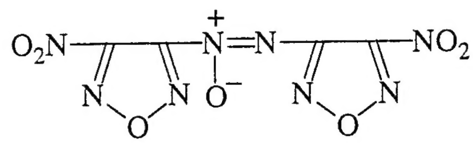
One of the compounds for which we have recently computed the gas phase heats of formation, ΔH_f(gaseous), is DNAF, **1** [1]. This was done using our density functional procedure [2].



DNAF, **1**

In response to interest expressed by the Air Force Armament Laboratory (Eglin AFB), we have now estimated the liquid and solid phase heats of formation of **1**. For this purpose, we needed the heats of vaporization, ΔH_{vap}, and sublimation, ΔH_{sub}, which we obtained using general correlations between these properties and computed quantities related to electrostatic potentials on molecular surfaces [3].

$$\Delta H_f(\text{liquid}) = \Delta H_f(\text{gaseous}) - \Delta H_{vap} \quad (1)$$

$$\Delta H_f(\text{solid}) = \Delta H_f(\text{gaseous}) - \Delta H_{sub} \quad (2)$$

We found ΔH_{vap} = 14 kcal/mole and ΔH_{sub} = 32 kcal/mole. Then,

$$\Delta H_f(\text{gaseous}) = 169 \text{ kcal/mole} = 621 \text{ cal/g}$$

$$\Delta H_f(\text{liquid}) = 155 \text{ kcal/mole} = 570 \text{ cal/g}$$

$$\Delta H_f(\text{solid}) = 137 \text{ kcal/mole} = 504 \text{ cal/g}$$

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1. P. Politzer and M. E. Grice, Technical Report No. 78, Office of Naval Research, Contract No. N00014-95-1-0028, March 16, 1995.
2. D. Habibollahzadeh, M. E. Grice, M. C. Concha, J. S. Murray and P. Politzer, J. Comp. Chem., **16**, 654 (1995).
3. M. DeSalvo, E. Miller, J. S. Murray and P. Politzer, unpublished work.